

# Harmonic oscillator eigenfunction expansions, quantum dots, and effective interactions

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We give a thorough analysis of the convergence properties of the configuration-interaction method as applied to parabolic quantum dots among other systems, including *a priori* error estimates. The method converges slowly in general, and in order to overcome this, we propose to use an effective two-body interaction well-known from nuclear physics. Through numerical experiments we demonstrate a significant increase in accuracy of the configuration interaction method.

## I. INTRODUCTION

The last two decades, an ever-increasing amount of research have been dedicated to understanding the electronic structure of so-called quantum dots<sup>1</sup>: semiconductor structures confining from a few to several thousands electrons in spatial regions on the nanometre scale. In such calculations, one typically seeks a few of the lowest eigenenergies  $E_k$  of the system Hamiltonian  $H$  and their corresponding eigenvectors  $\psi_k$ , i.e.,

$$H\psi_k = E_k\psi_k, \quad k = 1, \dots, k_{\max}. \quad (1.1)$$

One of the most popular methods is the (full) configuration interaction method (CI), where the many-body wave function is expanded in a basis of eigenfunctions of the harmonic oscillator (HO), and then necessarily truncated to give an approximation. In fact, the so-called curse of dimensionality implies that the number of degrees of freedom available per particle is severely limited. It is clear, that an understanding of the properties of such basis expansions is very important, as it is necessary for *a priori* error estimates of the calculations. Unfortunately, this is a neglected topic in the physics literature.

In this article, we give a thorough analysis of the (full) configuration interaction (CI) method using HO expansions applied to parabolic quantum dots, and give practical convergence estimates. It generalizes and refines the findings of a recent study of one-dimensional systems,<sup>2</sup> and is applicable to for example nuclear systems<sup>3</sup> and quantum chemical calculations<sup>4</sup> as well. We demonstrate the estimates with calculations in the  $d = 2$  dimensional case for  $N \leq 5$  electrons, paralleling computations in the literature<sup>5,6,7,8,9,10</sup>.

The main results are however somewhat discouraging. The expansion coefficients of typical eigenfunctions are shown to decay very slowly, limiting the accuracy of *any* practical method using HO basis functions. We therefore propose to use an effective two-body interaction to overcome, at least partially, the slow convergence rate. This is routinely used in nuclear physics<sup>3,11</sup> where the inter-particle forces are of a completely different, and basically unknown, nature. For electronic systems, however, the interaction is well-known and simpler to analyze, but effective interactions of the present kind have not been applied, at least to the author's knowledge. The modified method is seen to have convergence rates of at least one

order of magnitude higher than the original CI method. An important point here is that the complexity of the CI calculations is not altered, as no extra non-zero matrix elements are introduced. All one needs is a relatively simple one-time calculation to produce the effective interaction matrix elements.

The HO eigenfunctions are popular for several reasons. Many quantum systems, such as the quantum dot model considered here, are perturbed harmonic oscillators *per se*, so that the true eigenstates should be perturbations of the HO states. Moreover, the HO has many beautiful properties, such as complete separability of the Hamiltonian, invariance under orthogonal coordinate changes, and thus easily computed eigenfunctions, so that computing matrix elements of relevant operators becomes relatively simple. The HO eigenfunctions are defined on the *whole* of  $\mathbb{R}^d$  in which the particles live, so that truncation of the domain is unnecessary. Indeed, this is one of the main problems with methods such as finite difference or finite element methods.<sup>12</sup> On the other hand, the HO eigenfunctions are the *only* basis functions with all these properties.

The article is organized as follows. In Sec. II we discuss the harmonic oscillator and the the parabolic quantum dot model, including exact solutions for the  $N = 2$  case. In Sec. III, we give results for the approximation properties of the Hermite functions in  $n$  dimensions, and thus also of many-body HO eigenfunctions. By approximation properties, we mean estimates on the error  $\|\psi - P\psi\|$ , where  $\psi$  is any wave function and  $P$  projects onto a finite subspace of HO eigenfunctions, i.e., the model space. Here,  $P\psi$  is in fact the best approximation in the norm. The estimates will depend on analytic properties of  $\psi$ , i.e., whether it is differentiable, and whether it falls off sufficiently fast at infinity. To our knowledge, these results are not previously published.

In Sec. IV, we discuss the full configuration interaction method, using the results obtained in Sec. III to obtain convergence estimates of the method as function of the model space size. We also briefly discuss the effective interaction utilized in the numerical calculations, which are presented in Sec. V. We conclude with a discussion of the results, its consequences, and an outlook on further directions of research in Sec. VI.

We have also included an appendix with proofs of the formal propositions in Sec. III.

## II. THE HARMONIC OSCILLATOR AND PARABOLIC QUANTUM DOTS

### A. The Harmonic Oscillator

A spinless particle of mass  $m$  in an isotropic harmonic potential has Hamiltonian

$$H_{\text{HO}} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\|\vec{r}\|^2, \quad (2.1)$$

where  $\vec{r} \in \mathbb{R}^d$  is the particle's coordinates. By choosing proper energy and length units, i.e.,  $\hbar\omega$  and  $\sqrt{\hbar/m\omega}$ , respectively, the Hamiltonian becomes

$$H_{\text{HO}} = -\frac{1}{2}\nabla^2 + \frac{1}{2}\|\vec{r}\|^2. \quad (2.2)$$

$H_{\text{HO}}$  can be written as a sum over  $d$  one-dimensional harmonic oscillators, viz,

$$H_{\text{HO}} = \sum_{k=1}^d \left( -\frac{1}{2} \frac{\partial^2}{\partial r_k^2} + \frac{1}{2} r_k^2 \right), \quad (2.3)$$

so that a complete specification of the HO eigenfunctions is given by

$$\Phi_{\alpha_1, \alpha_2, \dots, \alpha_d}(\vec{r}) = \phi_{\alpha_1}(r_1) \phi_{\alpha_2}(r_2) \cdots \phi_{\alpha_d}(r_d), \quad (2.4)$$

where  $\phi_{\alpha_i}(x)$ ,  $\alpha_i = 0, 1, \dots$  are one-dimensional HO eigenfunctions, also called Hermite functions. These are defined by

$$\phi_n(x) = (2^n n! \pi^{1/2})^{-1/2} H_n(x) e^{-x^2/2}, \quad n = 0, 1, \dots, \quad (2.5)$$

where the Hermite polynomials  $H_n(x)$  are given by

$$H_n(x) = (-1)^n e^{x^2} \frac{\partial^n}{\partial x^n} e^{-x^2}. \quad (2.6)$$

The Hermite polynomials also obey the recurrence formula

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad (2.7)$$

with  $H_0(x) = 1$  and  $H_1(x) = 2x$ . The Hermite polynomial  $H_n(x)$  has  $n$  zeroes, and the Gaussian factor in  $\phi_n(x)$  will eventually subvert the polynomial for large  $|x|$ . Thus, qualitatively, the Hermite functions can be described as localized oscillations with  $n$  nodes and a Gaussian “tail” as  $x$  approaches  $\pm\infty$ . One can easily compute the quantum mechanical variance

$$(\Delta x)^2 := \int_{-\infty}^{\infty} x^2 \phi_n(x)^2 dx = n + \frac{1}{2}, \quad (2.8)$$

showing that, loosely speaking, the width of the oscillatory region increases as  $(n + 1/2)^{1/2}$ .

The functions  $\Phi_{\alpha_1, \dots, \alpha_d}$  defined in Eqn. (2.4) are called  $d$ -dimensional Hermite functions. In the sequel, we will define  $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathcal{I}_d$  for a tuple of non-negative

integers, also called a multi-index; see Appendix A 1. Using multi-indices, we may write

$$\Phi_{\alpha}(\vec{r}) = \left( 2^{|\alpha|} \alpha! \pi^{d/2} \right)^{-1/2} H_{\alpha_1}(r_1) \cdots H_{\alpha_d}(r_d) e^{-\|\vec{r}\|^2/2}. \quad (2.9)$$

The eigenvalue of  $\phi_n(x)$  is  $n + 1/2$ , so that the eigenvalue of  $\Phi_{\alpha}(\vec{r})$  is

$$\epsilon_{\alpha} = \frac{d}{2} + |\alpha|, \quad (2.10)$$

i.e., a zero-point energy  $d/2$  plus a non-negative integer. We denote by  $|\alpha|$  the *shell number* of  $\Phi_{\alpha}$ , and the eigenspace  $\mathcal{S}_r(\mathbb{R}^d)$  corresponding to the eigenvalue  $d/2 + r$  a *shell*. We define the *shell-truncated Hilbert space*  $\mathcal{P}_R(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$  as

$$\mathcal{P}_R(\mathbb{R}^d) := \text{span} \{ \Phi_{\alpha}(\vec{r}) \mid |\alpha| \leq R \} = \bigoplus_{r=0}^R \mathcal{S}_r(\mathbb{R}^d), \quad (2.11)$$

i.e., the subspace spanned by all Hermite functions with shell number less than or equal to  $R$ , or, equivalently, the direct sum of the shells up to and including  $R$ . The  $N$ -body generalization of this space, to be discussed in Section III B, is a very common model space used in CI calculations.

Since the Hermite functions constitute an orthonormal basis for  $L^2(\mathbb{R}^d)$ ,  $\mathcal{P}_R(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ , in the sense that for every  $\psi \in L^2(\mathbb{R}^d)$ ,  $\lim_{R \rightarrow \infty} \|\psi - P\psi\| = 0$ , where  $P$  is the orthogonal projector on  $\mathcal{P}_R(\mathbb{R}^d)$ . Strictly speaking, we should use a symbol like  $P_R$  or even  $P_R(\mathbb{R}^d)$  for the projector. However,  $R$  and  $d$  will always be clear from the context, so we are deliberately sloppy to obtain a concise formulation. For the same reason, we will sometimes simply write  $\mathcal{P}$  or  $\mathcal{P}_R$  for the space  $\mathcal{P}_R(\mathbb{R}^d)$ .

An important fact is that since  $H_{\text{HO}}$  is invariant under orthogonal spatial transformations (i.e., such transformation conserve energy), so is each individual shell space. Hence, each shell  $\mathcal{S}_r(\mathbb{R}^d)$ , and also  $\mathcal{P}_R(\mathbb{R}^d)$ , is independent of the spatial coordinates chosen.

For the case  $d = 1$  each shell  $r$  is spanned by a single eigenfunction, namely  $\phi_r(x)$ . For  $d = 2$ , each shell  $r$  has degeneracy  $r + 1$ , with eigenfunctions

$$\Phi_{(s, r-s)}(\vec{r}) = \phi_s(r_1) \phi_{r-s}(r_2), \quad 0 \leq s \leq r. \quad (2.12)$$

The usual HO eigenfunctions used to construct many-body wave functions are not the Hermite functions  $\Phi_{\alpha_1, \dots, \alpha_d}$ , however, but rather those obtained by utilizing the spherical symmetry of the HO. This gives a many-body basis diagonal in angular momentum. For  $d = 2$  we obtain the so-called Fock-Darwin orbitals given by

$$\Phi_{n,m}^{\text{FD}}(r, \theta) = \left[ \frac{2n!}{(n + |m|)!} \right]^{1/2} \frac{e^{im\theta}}{\sqrt{2\pi}} L_n^{|m|}(r^2) e^{-r^2/2}. \quad (2.13)$$

Here,  $n \geq 0$  is the nodal quantum number, counting the nodes of the radial part, and  $m$  is the azimuthal quantum

number. The eigenvalues are

$$\epsilon_{n,m} = 2n + |m| + 1. \quad (2.14)$$

Thus,  $R = 2n + |m|$  is the shell number. By construction, the Fock-Darwin orbitals are eigenfunctions of the angular momentum operator  $L_z = -i\partial/\partial\theta$  with eigenvalue  $m$ . Of course, we may write  $\Phi_{n,m}^{\text{FD}}$  as a linear combination of the Hermite functions  $\Phi_{(s,R-s)}$ , where  $0 \leq s \leq R = 2n + |m|$ , and vice versa. The actual choice of form of eigenfunctions is immaterial, as long as we may identify those belonging to a given shell.

The space  $\mathcal{P}_{R=4}(\mathbb{R}^2)$  is illustrated in Fig. 1 using both Hermite functions and Fock-Darwin orbitals.

### B. Parabolic quantum dots

We consider  $N$  electrons confined in a harmonic oscillator in  $d$  dimensions. This is a very common model for a quantum dot. We comment, that modelling the quantum dot geometry by a perturbed harmonic oscillator is justified by self-consistent calculations,<sup>13,14,15</sup> and is a widely adopted assumption.<sup>5,8,9,16,17,18</sup>

The Hamiltonian of the quantum dot is given by

$$H := T + U, \quad (2.15)$$

where  $T$  is the many-body HO Hamiltonian, given by

$$T = \sum_{k=1}^N H_{\text{HO}}(\vec{r}_k) \quad (2.16)$$

and  $U$  is the inter-electron Coulomb interactions. In dimensionless units the interaction is given by,

$$U := \sum_{i < j}^N C(i, j) = \sum_{i < j}^N \frac{\lambda}{\|\vec{r}_i - \vec{r}_j\|}. \quad (2.17)$$

The  $N$  electrons have coordinates  $\vec{r}_k$ , and the parameter  $\lambda$  measures the strength of the interaction over the confinement of the HO, viz,

$$\lambda := \frac{1}{\hbar\omega} \left( \frac{e^2}{4\pi\epsilon_0\epsilon} \right), \quad (2.18)$$

where we recall that  $\sqrt{\hbar/m\omega}$  is the length unit. Typical values for GaAs semiconductors are close to  $\lambda = 2$ , see for example Ref. 18. Increasing the trap size leads to a larger  $\lambda$ , and the quantum dot then approaches the classical regime.<sup>1</sup>

### C. Exact solution for two electrons

Before we discuss the approximation properties of the Hermite functions, it is instructive to consider the very simplest example of a two-electron parabolic quantum

dot and the properties of the eigenfunctions, since this case admits analytical solutions for special values of  $\lambda$  and is otherwise well understood<sup>19,20,21</sup>. Here, we consider  $d = 2$  dimensions only, but the  $d = 3$  case is similar. We note, that for  $N = 2$  it is enough to study the spatial wave function, since it must be either symmetric (for the singlet  $S = 0$  spin state) or anti-symmetric (for the triplet  $S = 1$  spin states). The Hamiltonian (2.15) becomes

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{1}{2}(r_1^2 + r_2^2) + \frac{\lambda}{r_{12}}, \quad (2.19)$$

where  $r_{12} = \|\vec{r}_1 - \vec{r}_2\|$  and  $r_j = \|\vec{r}_j\|$ . Introduce a set of scaled centre of mass coordinates given by  $\vec{R} = (\vec{r}_1 + \vec{r}_2)/\sqrt{2}$  and  $\vec{r} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2}$ . This coordinate change is orthogonal and symmetric in  $\mathbb{R}^4$ . This leads to the separable Hamiltonian

$$\begin{aligned} H &= -\frac{1}{2}(\nabla_r^2 + \nabla_R^2) + \frac{1}{2}(\|\vec{r}\|^2 + \|\vec{R}\|^2) + \frac{\lambda}{\sqrt{2}\|\vec{r}\|} \\ &= H_{\text{HO}}(\vec{R}) + H_{\text{rel}}(\vec{r}). \end{aligned}$$

A complete set of eigenfunctions of  $H$  can now be written on product form, viz,

$$\Psi(\vec{R}, \vec{r}) = \Phi_{n',m'}^{\text{FD}}(\vec{R})\psi(\vec{r}). \quad (2.20)$$

The relative coordinate wave function  $\psi(\vec{r})$  is an eigenfunction of the relative coordinate Hamiltonian given by

$$H_{\text{rel}} = -\frac{1}{2}\nabla_r^2 + \frac{1}{2}r^2 + \frac{\lambda}{\sqrt{2}r}, \quad (2.21)$$

where  $r = \|\vec{r}\|$ . This Hamiltonian can be further separated using polar coordinates, yielding eigenfunctions on the form

$$\psi_{m,n}(r, \theta) = \frac{e^{im\theta}}{\sqrt{2\pi}} u_{n,m}(r), \quad (2.22)$$

where  $|m| \geq 0$  is an integer and  $u_{n,m}$  is an eigenfunction of the radial Hamiltonian given by

$$H_r = -\frac{1}{2r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{|m|^2}{2r^2} + \frac{1}{2}r^2 + \frac{\lambda}{\sqrt{2}r}. \quad (2.23)$$

By convention,  $n$  counts the nodes away from  $r = 0$  of  $u_{n,m}(r)$ . Moreover, odd (even)  $m$  gives anti-symmetric (symmetric) wave functions  $\Psi(\vec{r}_1, \vec{r}_2)$ . For any given  $|m|$ , it is quite easy to deduce that the special value  $\lambda = \sqrt{2|m|+1}$  yields the eigenfunction

$$u_{0,m} = D r^{|m|} (a + r) e^{-r^2/2}, \quad (2.24)$$

where  $D$  and  $a$  are constants. The corresponding eigenvalue of  $H_r$  is  $E_r = |m| + 2$ , and  $E = 2n' + |m'| + 1 + E_r$ . Thus, the ground state (having  $m = m' = 0$ ,  $n = n' = 0$ ) for  $\lambda = 1$  is given by

$$\begin{aligned} \Psi_0(\vec{R}, \vec{r}) &= D(r + a) e^{-(r^2 + R^2)/2} \\ &= \frac{D}{\sqrt{2}} (r_{12} + \sqrt{2}a) e^{-(r_1^2 + r_2^2)/2}, \end{aligned}$$

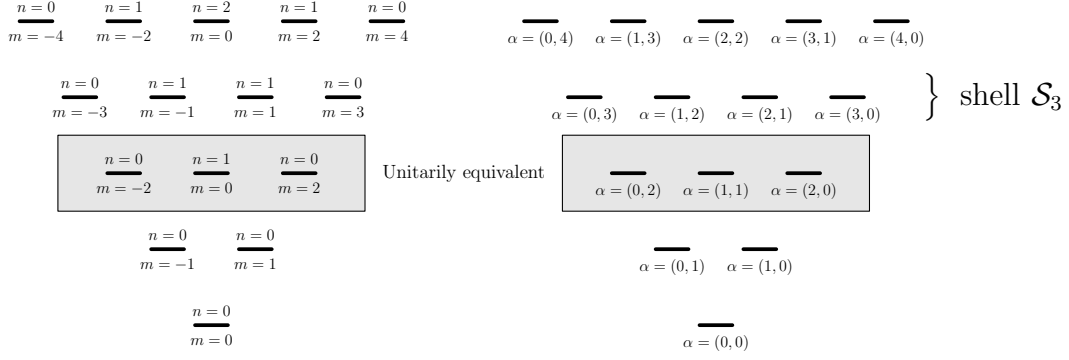


FIG. 1: Illustration of  $\mathcal{P}_{R=4}(\mathbb{R}^2)$ : (Left) Fock-Darwin orbitals. (Right) Hermite functions. Basis functions with equal HO energy are shown at same line.

with  $D$  being a (new) normalization constant.

Observe that this function has a cusp at  $r = 0$ , i.e., at the origin  $x = y = 0$  (where we have introduced Cartesian coordinates  $\vec{r} = (x, y)$  for the relative coordinate). Indeed, the partial derivatives  $\partial_x \psi_{0,0}$  and  $\partial_y \psi_{0,0}$  are not continuous there, and  $\Psi_0$  has no partial derivatives (in the distributional sense, see Appendix A 2) of second order. The cusp stems from the famous ‘‘cusp condition’’ which in simple terms states that, for a non-vanishing wave function at  $r_{12} = 0$ , the Coulomb divergence must be compensated by a similar divergence in the Laplacian.<sup>22,23</sup> This is only possible if the wave function has a cusp.

On the other hand, the non-smooth function  $\Psi_0(\vec{R}, \vec{r})$  is to be expanded in the HO eigenfunctions, e.g., Fock-Darwin orbitals. (Recall, that the particular representation for the HO eigenfunctions are immaterial – also whether we use lab coordinates  $\vec{r}_{1,2}$  or centre-of-mass coordinates  $\vec{R}$  and  $\vec{r}$ , since the coordinate change is orthogonal.) For  $m = 0$ , we have

$$\Phi_{n,0}^{\text{FD}}(r) = \sqrt{\frac{2}{\pi}} L_n(r^2) e^{-r^2/2}, \quad (2.25)$$

using the fact that these are independent of  $\theta$ . Thus,

$$\Psi_0(\vec{r}) = \Phi_{0,0}^{\text{FD}}(R) u_{0,0}(r) = \Phi_{0,0}^{\text{FD}}(R) \sum_{n=0}^{\infty} c_n \Phi_{n,0}^{\text{FD}}(r), \quad (2.26)$$

The functions  $\Phi_{n,0}^{\text{FD}}(r)$  are very smooth, as is seen by noting that  $L_n(r^2) = L_n(x^2 + y^2)$  is a polynomial in  $x$  and  $y$ , while  $u_{0,0}(r) = u_{0,0}(\sqrt{x^2 + y^2})$ , so Eqn. (2.26) is basically approximating a square root with a polynomial.

Consider then a truncated expansion  $\Psi_{0,R} \in \mathcal{P}_R(\mathbb{R}^2)$ , such as the one obtained with the CI or coupled cluster method.<sup>24</sup> In general, this is different from  $P_R \Psi_0$ , which is the best approximation of the wave function in  $\mathcal{P}_R(\mathbb{R}^2)$ . In any case, this expansion, consisting of the  $R + 1$  terms like those of Eqn. (2.26) is a very smooth function. Therefore, the cusp at  $r = 0$  cannot be well approximated.

In Section III C, we will show that the smoothness properties of the wave function  $\Psi$  is equivalent to a certain decay rate of the coefficients  $c_n$  in Eqn. (2.26) as  $n \rightarrow \infty$ . In this case, we will show that

$$\sum_{n=0}^{\infty} n^k |c_n|^2 < +\infty, \quad (2.27)$$

so that

$$|c_n| = o(n^{-(k+1+\epsilon)/2}). \quad (2.28)$$

Here,  $k$  is the number of times  $\Psi$  may be differentiated weakly, i.e.,  $\Psi \in H^k(\mathbb{R}^2)$ , and  $\epsilon \in [0, 1)$  is a constant. For the function  $\Psi_0$  we have  $k = 1$ . This kind of estimate directly tells us that an approximation using only a few HO eigenfunctions necessarily will give an error depending directly on the smoothness  $k$ .

We comment, that for higher  $|m|$  the eigenstates will still have cusps, albeit in the higher derivatives.<sup>22</sup> Indeed, we have weak derivatives of order  $|m| + 1$ , as can easily be deduced by operating on  $\psi_{0,m}$  with  $\partial_x$  and  $\partial_y$ . Moreover, recall that  $|m| = 1$  is the  $S = 1$  ground state, which then will have coefficients decaying faster than the  $S = 0$  ground state. Moreover, there will be excited states, i.e., states with  $|m| > 1$ , that also have more quickly decaying coefficients  $|c_n|$ . This will be demonstrated numerically in Sec. V.

In fact, Hoffmann-Ostenhof *et al.*<sup>22</sup> have shown that near  $r_{12} = 0$ , for arbitrary  $\lambda$  any local solution  $\Psi$  of  $(H - E)\Psi = 0$  has the form

$$\Psi(\xi) = \|\xi\|^m P\left(\frac{\xi}{\|\xi\|}\right) (1 + a\|\xi\|) + O(\|\xi\|^{m+1}), \quad (2.29)$$

where  $\xi = (\vec{r}_1, \vec{r}_2) \in \mathbb{R}^4$ , and where  $P$ ,  $\deg(P) = m$ , is a hyper-spherical harmonic (on  $S^3$ ), and where  $a$  is a constant. This also generalizes to arbitrary  $N$ , cf. Sec. III D. From this representation, it is manifest, that  $\Psi \in H^{m+1}(\mathbb{R}^4)$ , i.e.,  $\Psi$  has weak derivatives of order  $m + 1$ . We discuss these results further in Sec. III D.

### III. APPROXIMATION PROPERTIES OF HERMITE SERIES

#### A. Hermite functions in one dimension

In this section, we consider some formal mathematical propositions whose proofs are given in Appendix A 3, and discuss their importance for expansions in HO basis functions.

The first proposition considers the one-dimensional case, and the second considers general, multidimensional expansions. The latter result has to the author's knowledge not been published previously. The treatment for one-dimensional Hermite functions is similar, but not equivalent to, that given by Boyd<sup>25</sup> and Hille.<sup>26</sup>

We stress that the results are valid for *any* given wavefunction – not only eigenfunctions of quantum dot Hamiltonians – assuming only that the wavefunction decays exponentially as  $|x| \rightarrow \infty$ . In Appendix A 3, more general conditions are also considered.

The results are stated in terms of *weak* differentiability of the wavefunction, which is a generalization of the classical notion of a derivative. The space  $H^k(\mathbb{R}) \subset L^2(\mathbb{R})$  is roughly defined as the (square integrable) functions  $\psi(x)$  having  $k$  (square integrable) derivatives  $\partial_x^m \psi(x)$ ,  $0 \leq m \leq k$ . Correspondingly, the space  $H^k(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$  consists of the functions whose partial derivatives of total order  $\leq k$  are square integrable. For wavefunctions of electronic systems, it turns out that  $k$  times continuous differentiability implies  $k+1$  times weak differentiability<sup>22</sup>. The order  $k$  of differentiability is not always known, but an upper or lower bound can often be found through analysis. It is however important, that the Coulomb singularity implies that  $k$  is finite.

For the one-dimensional case, we have the following proposition:

**Proposition 1 (Approximation in one dimension)**  
Let  $k \geq 0$  be a given integer. Let  $\psi \in L^2(\mathbb{R})$  be exponentially decaying as  $|x| \rightarrow \infty$  and given by

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x), \quad (3.1)$$

where  $\phi_n(x)$  is given by Eqn. (2.5). Then  $\psi \in H^k(\mathbb{R})$  if and only if

$$\sum_{n=0}^{\infty} n^k |c_n|^2 < \infty. \quad (3.2)$$

We notice that the latter implies that

$$|c_n| = o(n^{-(k+1)/2}), \quad (3.3)$$

which shows that the more  $\psi(x)$  can be differentiated, the faster the coefficients will fall off as  $n \rightarrow \infty$ . Moreover, let  $\psi_R = P_R \psi = \sum_{n=0}^R c_n \phi_n$ . Then

$$\|\psi - \psi_R\| = \left( \sum_{n=R+1}^{\infty} |c_n|^2 \right)^{1/2}, \quad (3.4)$$

which gives an estimate of how well a finite basis of Hermite functions will approximate  $\psi(x)$  in the norm. We already notice, that for low  $k = 2$ , which is typical, the coefficients fall off as  $o(n^{-3/2})$ , which is rather slowly.

In the general  $n$ -dimensional case, the wavefunction  $\psi \in L^2(\mathbb{R}^n)$  has an expansion in the  $n$ -dimensional Hermite functions  $\Phi_\alpha(x)$ ,  $\alpha \in \mathcal{I}_n$  given by

$$\begin{aligned} \psi(x) &= \sum_{\alpha} c_{\alpha} \Phi_{\alpha}(x) \\ &= \sum_{\alpha_1 \dots \alpha_n} c_{\alpha_1 \dots \alpha_n} \phi_{\alpha_1}(x_1) \dots \phi_{\alpha_n}(x_n). \end{aligned}$$

In order to obtain useful estimates on the error, we need to define the *shell-weight*  $p(R)$  by the overlap of  $\psi(x)$  with the single shell  $\mathcal{S}_R$ , i.e.,

$$p(R) = \|P(\mathcal{S}_R)\psi\|^2 = \sum_{\alpha, |\alpha|=R} |c_{\alpha}|^2, \quad (3.5)$$

where  $P(\mathcal{S}_R)$  is the projection onto the shell. Thus,

$$\|\psi\|^2 = \sum_{R=0}^{\infty} p(R). \quad (3.6)$$

For the one-dimensional case, we of course have  $p(R) = |c_R|^2$ .

**Proposition 2 (Approximation in  $n$  dimensions)**  
Let  $\psi \in L^2(\mathbb{R}^n)$  be exponentially decaying as  $\|x\| \rightarrow \infty$  and given by

$$\psi(x) = \sum_{\alpha} c_{\alpha} \Phi_{\alpha}(x). \quad (3.7)$$

Then  $\psi \in H^k(\mathbb{R}^n)$  if and only if

$$\sum_{\alpha} |\alpha|^k |c_{\alpha}|^2 = \sum_{r=0}^{\infty} r^k p(r) < +\infty. \quad (3.8)$$

Again, we notice that the latter implies that

$$p(r) = o(r^{-(k+1)}). \quad (3.9)$$

Moreover, for the shell-truncated Hilbert space  $\mathcal{P}_R$ , the approximation error is given by

$$\|(1 - P)\psi\| = \left( \sum_{r=R+1}^{\infty} p(r) \right)^{1/2}. \quad (3.10)$$

In applications, we often observe a decay of non-integral order, i.e., there exists an  $\epsilon \in [0, 1)$  such that we observe

$$p(r) = o(r^{-(k+1+\epsilon)}). \quad (3.11)$$

This does not, of course, contradict the results. To see this, we observe that if  $\psi \in H^k(\mathbb{R}^n)$  but  $\psi \notin H^{k+1}(\mathbb{R}^n)$ , then  $p(r)$  must decay at least as fast as  $o(r^{-(k+1)})$  but

not as fast as  $o(r^{-k+2})$ . Thus, the actual decay exponent can be anything inside the interval  $[k+1, k+2]$ .

Consider also the case where  $\psi \in H^k(\mathbb{R}^n)$  for every  $k$ , i.e., we can differentiate it (weakly) as many times we like. Then  $p(r)$  decays faster than  $r^{-(k+1)}$ , for any  $k \geq 0$ , giving so-called exponential convergence of the Hermite series. Hence, functions that are best approximated by Hermite series are rapidly decaying *and* very smooth functions  $\psi$ . This would be the case for the quantum dot eigenfunctions if the inter-particle interactions were non-singular.

### B. Many-body wave functions

We now discuss  $N$ -body eigenfunctions of the HO in  $d$  dimensions, including spin, showing that we may identify the expansion of a such with  $2^N$  expansions in Hermite functions in  $n = Nd$  dimensions, i.e.,  $2^N$  expansions in HO eigenfunctions of imagined spinless particles in  $n = Nd$  dimensions. Each expansion corresponds to a different spin configuration.

Each particle  $k = 1, \dots, N$  has both spatial degrees of freedom  $\vec{r}_k \in \mathbb{R}^d$  and a spin coordinate  $\tau_k \in \{\pm 1\}$ , corresponding to the  $z$ -projection  $S_z = \pm \frac{\hbar}{2}$  of the electron spin. The configuration space can thus be taken as two copies  $X$  of  $\mathbb{R}^d$ ; one for each spin value, i.e.,  $X = \mathbb{R}^d \times \{\pm 1\}$  and  $x_k = (\vec{r}_k, \tau_k) \in X$  are the coordinates of particle  $k$ .

For a single particle with spin, the Hilbert space is now  $L^2(X)$ , with basis functions given by

$$\hat{\Phi}_i(x) = \Phi_\alpha(\vec{r})\chi_\sigma(\tau), \quad (3.12)$$

where  $i = i(\alpha, \sigma)$  is a new, generic index, and where  $\chi_\sigma$  is a basis function for the spinor space  $\mathbb{C}^2$ .

Ignoring the Pauli principle for the moment, the  $N$ -body Hilbert space is now given by

$$\mathcal{H}(N) = L^2(X)^N \equiv L^2(\mathbb{R}^{Nd}) \otimes (\mathbb{C}^2)^N, \quad (3.13)$$

i.e., each wavefunction  $\psi \in \mathcal{H}(N)$  is equivalent to  $2^N$  spin-component functions  $\psi^{(\sigma)} \in L^2(\mathbb{R}^{Nd})$ ,  $\sigma = (\sigma_1, \dots, \sigma_N) \in \{\pm 1\}^N$ . We have

$$\psi(x_1, \dots, x_N) = \sum_{\sigma} \psi^{(\sigma)}(\xi) \chi_{\sigma}(\tau), \quad \xi \equiv (\vec{r}_1, \dots, \vec{r}_N), \quad (3.14)$$

where  $\tau = (\tau_1, \dots, \tau_N)$ , and where  $\chi_{\sigma}(\tau) = \delta_{\sigma, \tau}$  are basis functions for the  $N$ -spinor space  $\mathbb{C}^{2^N}$ , being eigenfunctions for  $S_z$ , i.e., corresponding to a given configuration of the  $N$  spins.

The  $\sigma$ 'th component function  $\psi^{(\sigma)}(\xi) \in L^2(\mathbb{R}^{Nd})$  is a function of  $Nd$  variables, and by considering the  $Nd$ -dimensional HO as the sum of  $N$  HO's in  $d$  dimensions, it is easy to see that a basis for the  $L^2(\mathbb{R}^{Nd})$  is given by the functions

$$\Phi_{\beta}(\xi) \equiv \Phi_{\alpha^1}(\vec{r}_1) \cdots \Phi_{\alpha^N}(\vec{r}_N) \quad (3.15)$$

where  $\xi = (\vec{r}_1, \dots, \vec{r}_N)$ , and where  $\beta = (\alpha^1, \dots, \alpha^N)$  is an  $Nd$ -component multi-index. Correspondingly, a basis for the complete space  $\mathcal{H}(N) = L^2(X)^N$  is given by the functions

$$\hat{\Phi}_{i_1 \dots i_N}(\xi, \tau) \equiv \Phi_{\alpha^1}(\vec{r}_1) \cdots \Phi_{\alpha^N}(\vec{r}_N) \chi_{\sigma}(\tau), \quad (3.16)$$

where  $i_k = i(\alpha^k, \sigma_k)$ . Notice, that the HO energy and hence the shell number  $|\beta|$  only depends on  $\beta = (\alpha^1, \dots, \alpha^N)$ .

The functions  $\psi^{(\sigma)}$  may be expanded in the functions  $\Phi_{\beta}$ , i.e.,

$$\begin{aligned} \psi^{(\sigma)}(\xi) &= \sum_{\beta} c_{\beta}^{(\sigma)} \Phi_{\beta}(\xi) \\ &= \sum_{\alpha^1 \dots \alpha^N} c_{\alpha^1 \dots \alpha^N}^{(\sigma)} \Phi_{\alpha^1}(\vec{r}_1) \cdots \Phi_{\alpha^N}(\vec{r}_N), \end{aligned}$$

and we define the  $\sigma$ 'th shell weight  $p^{(\sigma)}(r)$  as before, i.e.,

$$p^{(\sigma)}(r) \equiv \sum_{|\beta|=r} |c_{\beta}^{(\sigma)}|^2. \quad (3.17)$$

We may then apply the analysis from Section III A to each of the spin component functions, and note that the *total* shell-weight is

$$p(r) \equiv \sum_{i_1 \dots i_N} \langle \hat{\Phi}_{i_1 \dots i_N}, \psi \rangle \delta_{|\beta|, r} = \sum_{\sigma} p^{(\sigma)}(r) \quad (3.18)$$

since the shell number  $|\beta| = \sum |\alpha_k|$  does not depend on the spin configuration of the basis function.

Including the Pauli principle to accommodate proper wave-function symmetry does not change these considerations. The basis functions  $\hat{\Phi}_{i_1 \dots i_N}$  are anti-symmetrized to become Slater determinants  $\Psi_{i_1 \dots i_N}$  (see for example Ref. 27 for details), which is equivalent to consider the projection  $\mathcal{H}_{AS}(N) = P_{AS} \mathcal{H}(N)$  of the unsymmetrized space onto the antisymmetric subspace. Moreover, the projections  $P_R$  and  $P_{AS}$  commute, so that the shell-truncated space is given by

$$\mathcal{P}_{AS, R} = \text{span} \left\{ \Psi_{i_1, \dots, i_N} : i_1 = i < \dots < i_N, \sum_k |\alpha^k| \leq R \right\}, \quad (3.19)$$

which is precisely the computational basis used in many CI calculations. (See however also the discussion in Section IV.) We stress, that,  $\mathcal{P}_{AS, R}$  is independent of the actual one-body HO eigenfunctions used. The shell-weight of  $\psi \in \mathcal{H}_{AS}(X)$  is now given by

$$p(r) = \sum_{i_1 \dots i_N} \langle \Psi_{i_1 \dots i_N}, \psi \rangle \delta_{|\beta(i_1 \dots i_N)|, r}, \quad (3.20)$$

and

$$\|P_R \psi\|^2 = \sum_{r=0}^R p(r). \quad (3.21)$$

As should be clear now, studying approximation of Hermite functions in arbitrary dimensions automatically gives the corresponding many-body HO approximation properties, since the many-body eigenfunctions can be seen as  $2^N$  component functions, and since the shell-truncated Hilbert space transfers to a many-body setting in a natural way.

### C. Two electrons revisited

We return to the exact solutions of the two-electron quantum dot considered in Sec. II C. Recall, that the wave functions were on the form

$$\psi(r, \theta) = e^{im\theta} f(r), \quad (3.22)$$

where  $f(r)$  decayed exponentially fast as  $r \rightarrow \infty$ . Assume now, that  $\psi \in H^k(\mathbb{R}^2)$ , i.e., that all partial derivatives of  $\psi$  of order  $k$  exists in the weak sense, viz,

$$\partial_x^j \partial_y^{k-j} \psi \in L^2(\mathbb{R}^2), \quad 0 \leq j \leq k, \quad (3.23)$$

where  $x = r \cos(\theta)$  and  $y = r \sin(\theta)$ . Then, by Lemma 4 in the Appendix,  $(a_x^\dagger)^j (a_y^\dagger)^{k-j} \psi \in L^2(\mathbb{R}^2)$  for  $0 \leq j \leq k$  as well.

The function  $\psi(r, \theta)$  was expanded in Fock-Darwin orbitals, viz,

$$\psi(r, \theta) = \sum_{n=0}^{\infty} c_n \Phi_{n,m}^{\text{FD}}(r, \theta). \quad (3.24)$$

Recall, that the shell number  $N$  for  $\Phi_{n,m}^{\text{FD}}$  was given by  $N = 2n + |m|$ . Thus, the shell-weight  $p(N)$  is in this case simply

$$p(N) = |c_{(N-|m|)/2}|^2, \quad N \geq |m|, \quad (3.25)$$

and  $p(N) = 0$  otherwise. From Prop. 2, we have

$$\sum_{N=|m|}^{\infty} N^k p(N) < +\infty, \quad (3.26)$$

which yields

$$|c_n| = o(n^{-(k+1+\epsilon)/2}), \quad 0 \leq \epsilon < 1, \quad (3.27)$$

as claimed in Sec. II C.

### D. Smoothness properties of many-electron wave functions

Let us mention some results, mainly due to Hoffmann-Ostenhof *et al.*,<sup>22,28</sup> concerning smoothness of many-electron wave functions. Strictly speaking, their results are valid only in  $d = 3$  spatial dimensions, since the Coulomb interaction in  $d = 2$  dimensions fails to be a Kato potential, the definition of which is quite subtle and

out of the scope for this article<sup>28</sup>. On the other hand, it is reasonable to assume that the results will still hold true, since the analytical results of the  $N = 2$  case is very similar in the  $d = 2$  and  $d = 3$  cases: The eigenfunctions decay exponentially with the same cusp singularities at the origin.<sup>19,20</sup>

Consider the Schrödinger equation  $(H - E)\psi(\xi) = 0$ , where  $\xi = (\xi_1, \dots, \xi_{Nd}) = (\vec{r}_1, \dots, \vec{r}_N) \in \mathbb{R}^{Nd}$ , and where  $\psi(\xi)$  is only assumed to be a solution locally. (A proper solution is of course also a local solution.) Recall, that  $\psi$  has  $2^N$  spin-components  $\psi^{(\sigma)}$ . Define a coalesce point  $\xi_{\text{CP}}$  as a point where at least two particles coincide, i.e.,  $\vec{r}_j = \vec{r}_\ell$ ,  $j \neq \ell$ . Away from the set of such points,  $\psi^{(\sigma)}(\xi)$  is real analytic, since the interaction is real analytic there. Near a  $\xi_{\text{CP}}$ , the wave function has the form

$$\psi^{(\sigma)}(\xi + \xi_{\text{CP}}) = r^k P(\xi/r)(1 + ar) + O(r^{k+1}), \quad (3.28)$$

where  $r = \|\xi\|$ ,  $P$  is a hyper-spherical harmonic (on the sphere  $S^{Nd-1}$ ) of degree  $k = k(\xi_{\text{CP}})$ , and where  $a$  is a constant. It is immediately clear, that  $\psi^{(\sigma)}(\xi)$  is  $k + 1$  times weakly differentiable in a neighborhood of  $\xi_{\text{CP}}$ . However, at  $K$ -electron coalesce points, i.e., at points  $\xi_{\text{CP}}$  where  $K$  different electrons coincide, the integer  $k$  may differ. Using exponential decay of a proper eigenfunction, we have  $\psi^{(\sigma)} \in H^{\min(k)+1}(\mathbb{R}^{Nd})$ . Hoffmann-Ostenhof *et al.* also showed, that symmetry restrictions on the spin-components due to the Pauli principle induces an increasing degree  $k$  of the hyper-spherical harmonic  $P$ , generating even higher order of smoothness. A general feature, is that the smoothness increases with the number of particles.

However, their results in this direction are not general enough to ascertain the *minimum* of the values for  $k$  for a given wave function, although we feel rather sure that such an analysis is possible. Suffice it to say, that the results are clearly visible in the numerical calculations in Sec. V.

Another interesting direction of research has been undertaken by Yserentant,<sup>29</sup> who showed that there are some very high order mixed partial derivatives at coalesce points. It seems unclear, though, if this can be exploited to improve the CI calculations further.

## IV. THE CONFIGURATION INTERACTION METHOD

### A. Convergence analysis using HO eigenfunction basis

The basic problem is to determine a few eigenvalues and eigenfunctions of the Hamiltonian  $H$  in Eqn. (2.15), i.e.,

$$H\psi_k = E_k\psi_k, \quad k = 1, \dots, k_{\text{max}}. \quad (4.1)$$

The CI method consists of approximating eigenvalues of  $H$  with those obtained by projecting the problem onto a

finite-dimensional subspace  $\mathcal{H}_h \subset \mathcal{H}(N)$ . As such, it is an example of the Ritz-Galerkin variational method.<sup>30,31</sup> We comment, that the convergence of the Ritz-Galerkin method is *not* simply a consequence of the completeness of the basis functions.<sup>30</sup> We will analyze the CI method when the model space is given by

$$\begin{aligned}\mathcal{H}_h &= P_R \mathcal{H}_{\text{AS}}(N) = \mathcal{P}_R(N) \\ &= \text{span} \left\{ \Psi_{i_1, \dots, i_N} : \sum_k |\alpha^k| \leq R \right\},\end{aligned}$$

used in Refs. 10,32, for example, although other spaces also are common. (We drop the subscript “AS” from now on.) The space

$$\mathcal{M}_R(N) := \text{span} \left\{ \Psi_{i_1, \dots, i_N} : \max_k |\alpha^k| \leq R \right\}, \quad (4.2)$$

i.e., a cut in the *single-particle* shell numbers (or energy) instead of the global shell number (or energy) is also common.<sup>6,8</sup> For obvious reasons,  $\mathcal{P}_R(N)$  is often referred to as an “energy cut space”, while  $\mathcal{M}_R(N)$  is referred to as a “direct product space”.

As in Sec. III A,  $P_R$  is the orthogonal projector onto the model space  $\mathcal{P}_R(N)$ . We also define  $Q_R = 1 - P_R$  as the projector onto the excluded space  $\mathcal{P}_R(N)^\perp$ . The discrete eigenvalue problem is then

$$(P_R H P_R) \psi_{h,k} = E_{h,k} \psi_{h,k}, \quad k = 1, \dots, k_{\text{max}}. \quad (4.3)$$

The CI method becomes, in principle, exact as  $R \rightarrow \infty$ . Indeed, a widely-used name for the CI method is “exact diagonalization,” being somewhat a misnomer as only a very limited number of degrees of freedom per particle is achievable.

It is clear that

$$\mathcal{P}_R(N) \subset \mathcal{M}_R(N) \subset \mathcal{P}_{NR}(N), \quad (4.4)$$

so that studying the convergence in terms of  $\mathcal{P}_R(N)$  is sufficient. In our numerical experiments we therefore focus on the energy cut model space. A comparison between the convergence of the two spaces is, on the other hand, an interesting topic for future research.

Using the results in Refs. 30,33 for non-degenerate eigenvalues for simplicity, we obtain an estimate for the error in the numerical eigenvalue  $E_h$  as

$$E_h - E \leq [1 + \nu(R)](1 + K\lambda) \langle \psi, Q_R T \psi \rangle, \quad (4.5)$$

where  $K$  is a constant, and where  $\nu(R) \rightarrow 0$  as  $R \rightarrow \infty$ . Using  $T\Phi_\beta = (Nd/2 + |\beta|)\Phi_\beta$  and Eqn. (3.8), we obtain

$$\langle \psi, Q_R T \psi \rangle = \sum_{r=R+1}^{\infty} \left( \frac{Nd}{2} + r \right) p(r). \quad (4.6)$$

Assume now, that  $\psi^{(\sigma)} \in H^k(\mathbb{R}^{Nd})$  for all  $\sigma$ , so that according to Proposition 2, we will have

$$\sum_{r=0}^{\infty} r^k p(r) < +\infty \quad (4.7)$$

implying that  $rp(r) = o(r^{-k})$ . We then obtain, for  $k > 1$ ,

$$\langle \psi, (1 - P_R) T \psi \rangle = o(R^{-(k-1)}) + o(R^{-k}). \quad (4.8)$$

For  $k = 1$  (which is the worst case), we merely obtain convergence,  $\langle \psi, (1 - P_R) T \psi \rangle \rightarrow 0$  as  $R \rightarrow \infty$ . We assume, that  $R$  is sufficiently large, so that the  $o(R^{-k})$  term can be neglected.

Again, we may observe a slight deviation from the decay, and we expect to observe eigenvalue errors on the form

$$E_h - E \sim (1 + K\lambda) R^{-(k-1+\epsilon)}, \quad (4.9)$$

where  $0 \leq \epsilon < 1$ .

As for the eigenvector error  $\|\psi_h - \psi\|$  (recall that  $\psi_h \neq P_R \psi$ ), we mention that

$$\|\psi_h - \psi\| \leq [1 + \eta(R)] [(1 + K\lambda) \langle \psi, (1 - P_R) T \psi \rangle]^{1/2}, \quad (4.10)$$

where  $\eta(R) \rightarrow 0$  as  $R \rightarrow \infty$ .

## B. Effective interaction scheme

Effective interactions have a long tradition in nuclear physics, where the bare nuclear interaction is basically unknown and highly singular, and where it must be renormalized and fitted to experimental data.<sup>3</sup> In quantum chemistry and atomic physics, the Coulomb interaction is of course well-known so there is no intrinsic need to formulate an effective interaction. However, in lieu of the in general low order of convergence implied by Eqn. (4.9), we believe that HO-based calculations like the CI method in general may benefit from the use of effective interactions.

A complete account of the effective interaction scheme outlined here is out of scope for the present article, but we refer to Refs. 2,11,34,35,36 for details as well as numerical algorithms.

Recall, that the interaction is given by

$$U = \sum_{i < j}^N C(i, j) = \sum_{i < j}^N \frac{\lambda}{\|\vec{r}_i - \vec{r}_j\|}, \quad (4.11)$$

a sum of fundamental two-body interactions. For the  $N = 2$  problem we have in principle the exact solution, since the Hamiltonian (2.19) can be reduced to a one-dimensional radial equation, e.g., the eigenproblem of  $H_r$  defined in Eqn. (2.21). This equation may be solved to arbitrarily high precision using various methods, for example using a basis expansion in generalized half-range Hermite functions.<sup>37</sup> In nuclear physics, a common approach is to take the best two-body CI calculations available, where  $R = O(10^3)$ , as “exact” for this purpose.

We now define the effective Hamiltonian for  $N = 2$  as a Hermitian operator  $H_{\text{eff}}$  defined only within  $\mathcal{P}_R(N = 2)$  that gives  $K = \dim[\mathcal{P}_R(N = 2)]$  *exact* eigenvalues  $E_k$



of  $H$ , and  $K$  approximate eigenvectors  $\psi_{\text{eff},k}$ . Of course, there are infinitely many choices for the  $K$  eigenpairs, but by treating  $U = \lambda/r_{12}$  as a perturbation, and “following” the unperturbed HO eigenpairs ( $\lambda = 0$ ) through increasing values of  $\lambda$ , one makes the eigenvalues unique.<sup>2,38</sup> The approximate eigenvectors  $\psi_{\text{eff},k} \in \mathcal{P}_R(N = 2)$  are chosen by minimizing the distance to the exact eigenvectors  $\psi_k \in \mathcal{H}(N = 2)$  while retaining orthonormality.<sup>35</sup> This uniquely defines  $H_{\text{eff}}$  for the two-body system. In terms of matrices, we have

$$H_{\text{eff}} = \tilde{U} \text{diag}(E_1, \dots, E_K) \tilde{U}^\dagger, \quad (4.12)$$

where  $X$  and  $Y$  are unitary matrices defined as follows. Let  $U$  be the  $K \times K$  matrix whose  $k$ 'th column is the coefficients of  $P_R \psi_k$ . Then the singular value decomposition of  $U$  can be written

$$U = X \Sigma Y^\dagger, \quad (4.13)$$

where  $\Sigma$  is diagonal. Then,

$$\tilde{U} := X Y^\dagger. \quad (4.14)$$

The columns of  $\tilde{U}$  are the projections  $P_R \psi_k$  “straightened out” to an orthonormal set. Eqn. (4.12) is simply the spectral decomposition of  $H_{\text{eff}}$ . Although different in form than most implementations in the literature (e.g., Ref. 11), it is equivalent.

The effective two-body interaction  $C_{\text{eff}}(i, j)$  is now given by

$$C_{\text{eff}}(1, 2) := H_{\text{eff}} - P_R T P_R, \quad (4.15)$$

which is defined only within  $\mathcal{P}_R(N = 2)$ .

The  $N$ -body effective Hamiltonian is defined by

$$H_{\text{eff}} := P_R T P_R + \sum_{i < j}^N C_{\text{eff}}(i, j), \quad (4.16)$$

where  $P_R$  projects onto  $\mathcal{P}_R(N)$ , and thus  $H_{\text{eff}}$  is defined *only* within  $\mathcal{P}_R(N)$ . The diagonalization of  $H_{\text{eff}}(N)$  is equivalent to a perturbation technique where a certain class of diagrams is summed to infinite order in the full problem.<sup>34</sup> In implementations, (4.12) and (4.16) are treated in COM coordinates, utilizing block diagonality of both  $H$  and  $H_{\text{eff}}$ , see Ref. 36 for details.

We comment that unlike the bare Coulomb interaction, the effective two-body interaction  $C_{\text{eff}}$  corresponds to a non-local potential due to the “straightening out” of truncated eigenvectors.

Rigorous mathematical treatment of the convergence properties of the effective interaction is, to the author’s knowledge, not available. Effective interactions have, however, enjoyed great success in the nuclear physics community, and we strongly believe that we soon will see sufficient proof of the improved accuracy with this method. Indeed, in Sec. V we see clear evidence of the accuracy boost when using an effective interaction.

## V. NUMERICAL RESULTS

### A. Code description

We now present numerical results using the full configuration-interaction method for  $N = 2$ –5 electrons in  $d = 2$  dimensions. We will use both the “bare” Hamiltonian  $H = T + U$  and the effective Hamiltonian (4.16).

Since the Hamiltonian commutes with angular momentum  $L_z$ , the latter taking on eigenvalues  $M \in \mathbb{Z}$ , the Hamiltonian matrix is block diagonal. (Recall, that the Fock-Darwin orbitals  $\Phi_{n,m}^{\text{FD}}$  are eigenstates of  $L_z$  with eigenvalue  $m$ , so each Slater determinant has eigenvalue  $M = \sum_{k=1}^N m_k$ .) Moreover, the calculations are done in a basis of joint eigenfunctions for total electron spin  $S^2$  and its projection  $S_z$ , as opposed to the Slater determinant basis used for convergence analysis. Such basis functions are simply linear combinations of Slater determinants within the same shell, and further reduce the dimensionality of the Hamiltonian matrix.<sup>8</sup> The eigenfunctions of  $H$  are thus labeled with the total spin  $S = 0, 1, \dots, \frac{N}{2}$  for even  $N$  and  $S = \frac{1}{2}, \frac{3}{2}, \dots, \frac{N}{2}$  for odd  $N$ , as well as the total angular momentum  $M = 0, 1, \dots$  ( $-M$  produce the same eigenvalues as  $M$ , by symmetry.) We thus split  $\mathcal{P}_R(N)$  (or  $\mathcal{M}_R(N)$ ) into invariant subspaces  $\mathcal{P}_R(N, M, S)$  ( $\mathcal{M}_R(N, M, S)$ ) and perform computations solely within these.

The calculations were carried out with a code similar to that described by Rontani *et al.* in Ref. 8. Table I shows comparisons of the present code with that of Table IV of Ref. 8 for various parameters using the model space  $\mathcal{M}_R(N, M, S)$ . Table I also shows the case  $\lambda = 1$ ,  $N = 2$ ,  $M = 0$ , and  $S = 0$ , whose exact lowest eigenvalue is  $E_0 = 3$ , cf. Sec. II C. We note that there are some discrepancies between the results in the last digits of the results of Ref. 8. The spaces  $\mathcal{M}_R(N)$  were identical in the two approaches, i.e., the number of basis functions and the number of non-zero matrix elements produced are cross-checked and identical.

We have checked that the code also reproduces the results of Refs. 9, 10, 39, using the  $\mathcal{P}_R(N, M, S)$  spaces. Our code is described in detail elsewhere<sup>36</sup> where it is also demonstrated that it reproduces the eigenvalues of an analytically solvable  $N$ -particle system<sup>40</sup> to machine precision.

### B. Experiments

For the remainder, we only use the energy cut spaces  $\mathcal{P}_R(N, M, S)$ . Figure 2 shows the development of the lowest eigenvalue  $E_0 = E_0(N, M, S)$  for  $N = 4$ ,  $M = 0, 1, 2$  and  $S = 0$  as function of the shell truncation parameter  $R$ , using both Hamiltonians  $H$  and  $H_{\text{eff}}$ . Apparently, the effective interaction eigenvalues provide estimates for the ground state eigenvalues that are better than the bare interaction eigenvalues. This effect is attenuated

TABLE I: Comparison of current code and Ref. 8. Figures from the latter have varying number of significant digits. We include more digits from our own computation for reference

$N$	$\lambda$	$M$	$2S$	$R = 5$		$R = 6$		$R = 7$	
				Current	Ref. 8	Current	Ref. 8	Current	Ref. 8
2	1	0	0	3.013626		3.011020		3.009236	
	2	0	0	3.733598	3.7338	3.731057	3.7312	3.729324	3.7295
		1	2	4.143592	4.1437	4.142946	4.1431	4.142581	4.1427
3	2	1	1	8.175035	8.1755	8.169913		8.166708	8.1671
	4	1	1	11.04480	11.046	11.04338		11.04254	11.043
		0	3	11.05428	11.055	11.05325		11.05262	11.053
4	6	0	0	23.68944	23.691	23.65559		23.64832	23.650
		2	4	23.86769	23.870	23.80796		23.80373	23.805
5	2	0	5	21.15093	21.15	21.13414	21.13	21.12992	21.13
	4	0	5	29.43528	29.44	29.30898	29.31	29.30251	29.30

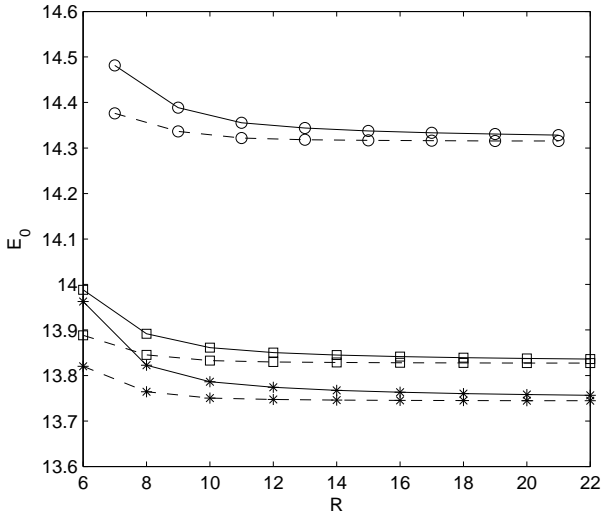


FIG. 2: Eigenvalues for  $N = 4$ ,  $S = 0$ ,  $\lambda = 2$  as function of  $R$  for  $H$  (solid) and  $H_{\text{eff}}$  (dashed).  $M = 0, 1$  and  $2$  are represented by squares, circles and stars, resp.

with higher  $N$ , due to the fact that the two-electron effective Coulomb interaction does not take into account three- and many-body effects which become substantial for higher  $N$ .

We take the  $H_{\text{eff}}$ -eigenvalues as “exact” and graph the relative error in  $E_0(N, M, S)$  as function of  $R$  on a logarithmic scale in Fig. 3, in anticipation of the relation

$$\ln(E_h - E) \approx C + \alpha \ln R, \quad \alpha = -(k - 1 + \epsilon). \quad (5.1)$$

The graphs show straight lines for large  $R$ , while for small  $R$  there is a transient region of non-straight lines. For  $N = 5$ , however,  $\lambda = 2$  is too large a value to reach the linear regime for the range of  $R$  available, so in this case we chose to plot the corresponding error for the very small value  $\lambda = 0.2$ , showing clear straight lines in the error. The slopes are more or less independent of  $\lambda$ , as observed in different calculations.

In Fig. 4 we show the corresponding graphs when using the effective Hamiltonian  $H_{\text{eff}}$ . We estimate the relative error as before, leading to artifacts for the largest values of  $R$  due to the fact that there is a finite error in the best estimates for the eigenvalues. However, in all cases there are clear, linear regions, in which we estimate the slope  $\alpha$ . In all cases, the slope can be seen to decrease by at least  $\Delta\alpha \approx -1$  compared to Fig. 3, indicating that the effective interaction indeed accelerates the CI convergence by at least an order of magnitude. We also observe, that the relative errors are improved by an order of magnitude or more for the lowest values of  $R$  shown, indicating the gain in accuracy when using small model spaces with the effective interaction.

Notice, that for symmetry reasons only even (odd)  $R$  for even (odd)  $M$  yields increases in basis size  $\dim[\mathcal{P}_R(N, M, S)]$ , so only these values are included in the plots.

To overcome the limitations of the two-body effective interaction for higher  $N$ , an effective three-body interaction could be considered, and is hotly debated in the nuclear physics community. (In nuclear physics, there are also more complicated three-body effective forces that need to be included.<sup>41</sup>) However, this will lead to a huge increase in memory consumption due to extra nonzero matrix elements. At the moment, there are no methods available that can generate the exact three-body effective interaction with sufficient precision.

We stress, that the relative error decreases very slowly in general. It is a common misconception, that if a number of digits of  $E_0(N, M, S)$  is unchanged between  $R$  and  $R + 2$ , then these digits have converged. This is not the case, as is easily seen from Fig. 3. Take for instance  $N = 4$ ,  $M = 0$  and  $S = 0$ , and  $\lambda = 2$ . For  $R = 14$  and  $R = 16$  we have  $E_0 = 13.84491$  and  $E_0 = 13.84153$ , respectively, which would give a relative error estimate of  $2.4 \times 10^{-4}$ , while the correct relative error is  $1.3 \times 10^{-3}$ .

The slopes in Fig. 3 vary greatly, showing that the eigenfunctions indeed have varying global smoothness, as predicted in Sec. III D. For  $(N, M, S) = (5, 3, 5/2)$ , for example,  $\alpha \approx -4.2$ , indicating that  $\psi \in H^5(\mathbb{R}^{10})$ . It seems, that higher  $S$  gives higher  $k$ , as a rule of thumb.

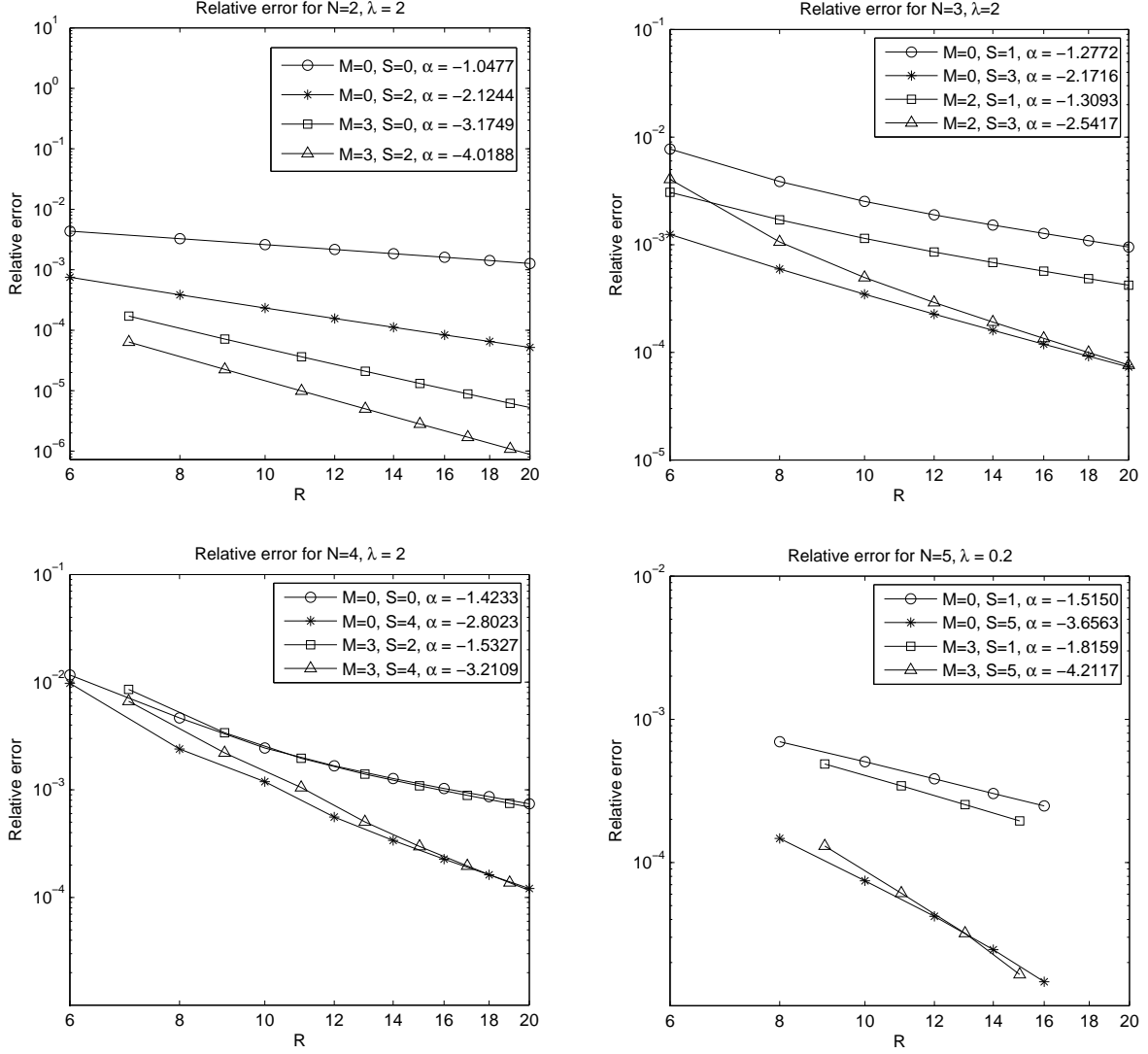


FIG. 3: Plot of relative error using the bare interaction for various  $N$ ,  $M$  and  $S$ . Clear  $o(R^\alpha)$  dependence in all cases.

Intuitively, this is because the Pauli principle forces the wave function to be zero at coalesce points, thereby generating smoothness.

## VI. DISCUSSION AND CONCLUSION

We have studied approximation properties of Hermite functions and harmonic oscillator eigenfunctions. This in turn allowed for a detailed convergence analysis of numerical methods such as the CI method for the parabolic quantum dot. Our main conclusion, is, that for wave functions  $\psi \in H^k(\mathbb{R}^n)$  falling off exponentially as  $\|x\| \rightarrow \infty$ , the shell-weight function  $p(r)$  decays as  $p(r) = o(r^{-k-1})$ . Applying this to the convergence theory of the Ritz-Galerkin method, we obtained the estimate (4.5) for the error in the eigenvalues. A complete characterization of the upper bound on the differentia-

bility  $k$ , i.e., in  $\psi^{(s)} \in H^k$ , as well as a study of the constant  $K$  in Eqn. (4.9), would complete our knowledge of the convergence of the CI calculations.

We also demonstrated numerically, that the use of a two-body effective interaction accelerates the convergence by at least an order of magnitude, which shows that such a method *should* be used whenever possible. On the other hand, a rigorous mathematical study of the method is yet to come. Moreover, we have not investigated to what extent the increase in convergence is independent of the interaction strength  $\lambda$ . This, together with a study of the accuracy of the *eigenvectors*, is an obvious candidate for further investigation.

The theory and ideas presented in this article should in principle be universally applicable. In fact, Figs. 1–3 of Ref. 11 clearly indicates this, where the eigenvalues of  $^3\text{He}$  as function of model space size are graphed both for bare and effective interactions, showing some of the

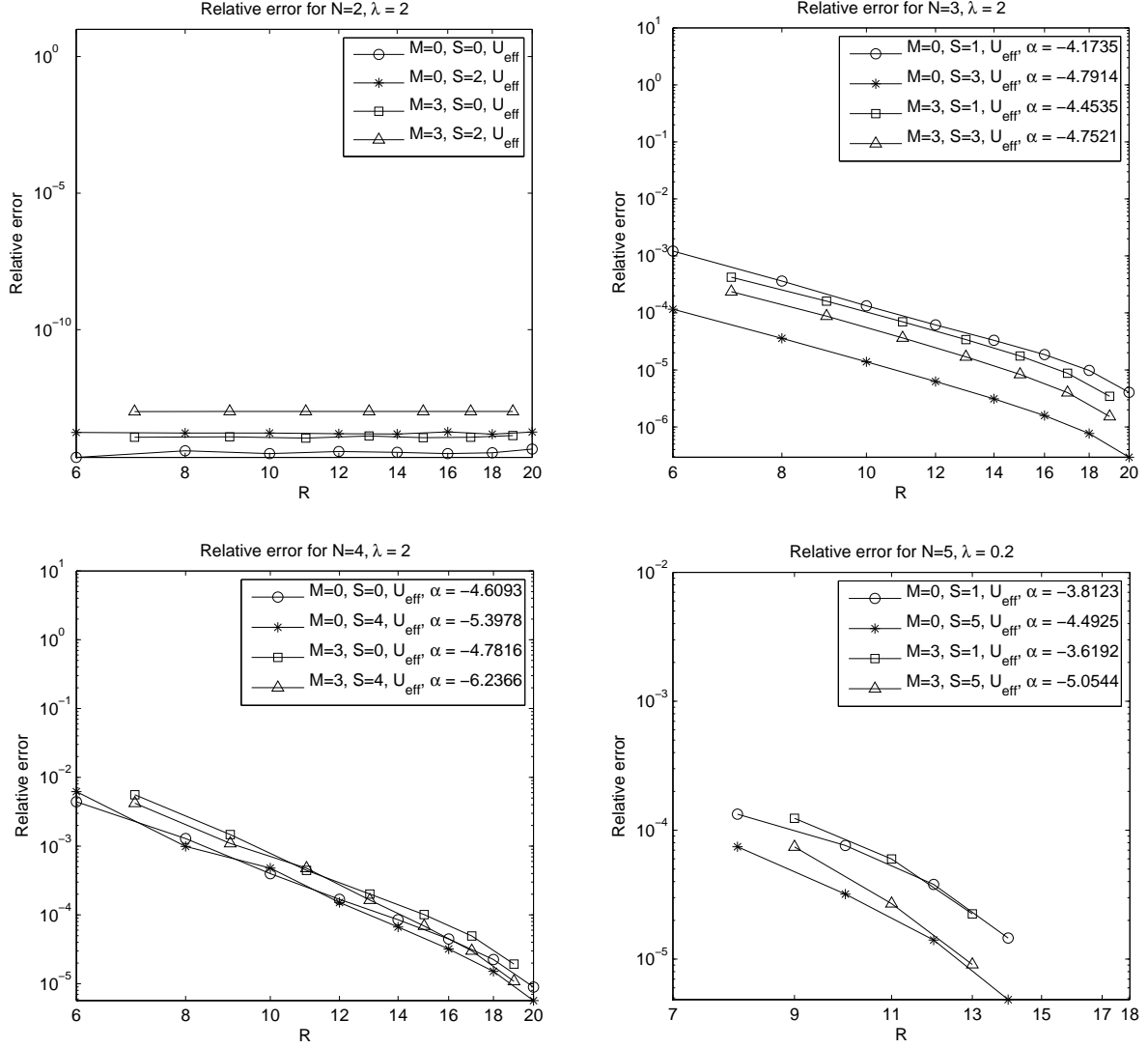


FIG. 4: Plot of relative error using an effective interaction for various  $N$ ,  $M$  and  $S$ . Clear  $o(R^\alpha)$  dependence in all cases, but notice artifacts when  $R$  is large, due to errors in most correct eigenvalues. The  $R = 5$  case does not contain enough data to compute the slopes with sufficient accuracy.

features we have discussed.

Other interesting future studies would be a direct comparison of the direct product model space  $\mathcal{M}_R(N)$  and our energy cut model space  $\mathcal{P}_R(N)$ . Both techniques are common, but may have different numerical characteristics. Indeed,  $\dim[\mathcal{M}_R(N)]$  grows much quicker than  $\dim[\mathcal{P}_R(N)]$ , while we are uncertain of whether the increased basis size yields a corresponding increased accuracy.

We have focused on the parabolic quantum dot, firstly because it requires relatively small matrices to be stored, due to conservation of angular momentum, but also because it is a widely studied model. Our analysis is, however, general, and applicable to other systems as well, e.g., quantum dots trapped in double-wells, finite wells, and so on. Indeed, by adding a one-body potential  $V$

to the Hamiltonian  $H = T + U$  we may model other geometries, as well as adding external fields.<sup>42,43,44</sup>

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## APPENDIX A: MATHEMATICAL DETAILS

### 1. Multi-indices

A very handy tool for compact and unified notation when the dimension  $n$  of the underlying measure space  $\mathbb{R}^n$  is a parameter, are multi-indices. The set  $\mathcal{I}_n$  of multi-indices are defined as  $n$ -tuples of non-negative indices, viz,  $\alpha = (\alpha_1, \dots, \alpha_n)$ , where  $\alpha_k \geq 0$ .

We define several useful operations on multi-indices as follows. Let  $u$  be a formal vector of  $n$  symbols. Moreover, let  $\phi(\xi) = \phi(\xi_1, \xi_2, \dots, \xi_n)$  be a function. Then, define

$$|\alpha| \equiv \alpha_1 + \alpha_2 + \dots + \alpha_n \quad (\text{A.1})$$

$$\alpha! \equiv \alpha_1! \alpha_2! \dots \alpha_n! \quad (\text{A.2})$$

$$\alpha \pm \beta \equiv (\alpha_1 \pm \beta_1, \dots, \alpha_n \pm \beta_n) \quad (\text{A.3})$$

$$u^\alpha \equiv u_1^{\alpha_1} u_2^{\alpha_2} \dots u_n^{\alpha_n}, \quad (\text{A.4})$$

$$\partial^\alpha \phi(\xi) \equiv \frac{\partial^{\alpha_1}}{\partial \xi_1^{\alpha_1}} \frac{\partial^{\alpha_2}}{\partial \xi_2^{\alpha_2}} \dots \frac{\partial^{\alpha_d}}{\partial \xi_d^{\alpha_d}} \phi(\xi) \quad (\text{A.5})$$

In Eqn. (A.3), the result may not be a multi-index when we subtract two indices, but this will not be an issue for us. Notice, that Eqn. (A.5) is a mixed partial derivative of order  $|\alpha|$ . Moreover, we say that  $\alpha < \beta$  if and only if  $\alpha_j < \beta_j$  for all  $j$ . We define  $\alpha = \beta$  similarly. We also define “basis indices”  $e_j$  by  $(e_j)_{j'} = \delta_{j,j'}$ . We comment, that we will often use the notation  $\partial_x \equiv \frac{\partial}{\partial x}$  and  $\partial_k \equiv \frac{\partial}{\partial \xi_k}$  to simplify notation. Thus,

$$\partial^\alpha = (\partial_1^{\alpha_1}, \dots, \partial_n^{\alpha_n}), \quad (\text{A.6})$$

consistent with Eqn. (A.4).

### 2. Weak derivatives and Sobolev spaces

We present a quick summary of weak derivatives and related concepts needed. The material is elementary and superficial, but probably unfamiliar to many readers, so we include it here. Many terms will be left undefined; if needed, the reader may consult standard texts, e.g., Ref. 45.

The space  $L^2(\mathbb{R}^n)$  is defined as

$$L^2(\mathbb{R}^n) \equiv \left\{ \psi : \mathbb{R}^n \rightarrow \mathbb{C} : \int_{\mathbb{R}^n} |\psi(\xi)|^2 d^n \xi < +\infty \right\}, \quad (\text{A.7})$$

where the Lebesgue integral is more general than the Riemann “limit-of-small-boxes” integral. It is important that we identify two functions  $\psi$  and  $\psi_1$  differing only at a set  $Z \in \mathbb{R}^n$  of measure zero. Examples of such sets are points if  $n \geq 1$ , curves if  $n \geq 2$ , and so on, and countable unions of such. For example, the rationals constitute a set of measure zero in  $\mathbb{R}$ . Under this assumption,  $L^2(\mathbb{R}^n)$  becomes a Hilbert space with the inner product

$$\langle \psi_1, \psi_2 \rangle \equiv \int_{\mathbb{R}^n} \psi_1(\xi)^* \psi_2(\xi) d^n \xi, \quad (\text{A.8})$$

where the asterisk denotes complex conjugation.

The classical derivative is too limited a concept for the abstract theory of partial differential equations, including the Schrödinger equation. Let  $\mathcal{C}_0^\infty$  be the set of infinitely differentiable functions which are non-zero only in a ball of finite radius. Of course,  $\mathcal{C}_0^\infty \subset L^2(\mathbb{R}^n)$ . Let  $\psi \in L^2(\mathbb{R}^n)$ , and let  $\alpha \in \mathcal{I}_n$  be a multi-index. If there exists a  $v \in L^2(\mathbb{R}^n)$  such that, for all  $\phi \in \mathcal{C}_0^\infty$ ,

$$\int_{\mathbb{R}^n} (\partial^\alpha \phi(\xi)) \psi(\xi) d^n \xi = (-1)^{|\alpha|} \int_{\mathbb{R}^n} \phi(\xi) v(\xi) d^n \xi, \quad (\text{A.9})$$

then  $\partial^\alpha \psi \equiv v \in L^2$  is said to be a *weak derivative*, or *distributional derivative*, of  $\psi$ . In this way, the weak derivative is defined in an average sense, using integration by parts.

The weak derivative is unique (up to redefinition on a set of measure zero), obeys the product rule, chain rule, etc.

It is easily seen, that if  $\psi$  has a classical derivative  $v \in L^2(\mathbb{R}^n)$  it coincides with the weak derivative. Moreover, if the classical derivative is defined almost everywhere (i.e., everywhere except for a set of measure zero), then  $\psi$  has a weak derivative.

The Sobolev space  $H^k(\mathbb{R}^n)$  is defined as the subset of  $L^2(\mathbb{R}^n)$  given by

$$H^k(\mathbb{R}^n) \equiv \{ \psi \in L^2 : \partial^\alpha \psi \in L^2, \quad \forall \alpha \in \mathcal{I}_n, |\alpha| \leq k \}. \quad (\text{A.10})$$

The Sobolev space is also a Hilbert space with the inner product

$$\langle \psi_1, \psi_2 \rangle \equiv \sum_{\alpha, |\alpha| \leq k} \langle \partial^\alpha \psi_1, \partial^\alpha \psi_2 \rangle, \quad (\text{A.11})$$

and this is the main reason why one obtains a unified theory of partial differential equations using such spaces.

The space  $H^k(\mathbb{R}^n)$  for  $n > 1$  is a big space – there are some exceptionally ill-behaved functions there, for example there are functions in  $H^k$  that are unbounded on arbitrary small regions but still differentiable. (Hermite series for such functions would still converge faster than, e.g., for a function with a jump discontinuity!) For our purposes, it is enough to realize that the Sobolev spaces offer exactly the notion of derivative we need in our analysis of the Hermite function expansions.

### 3. Proofs of propositions

We will now prove the propositions given in Sec. III, and also discuss these results on mathematical terms.

Recall that the Hermite functions  $\phi_n \in L^2(\mathbb{R})$ , where  $n \in \mathbb{N}_0$  is a non-negative integer, are defined by

$$\phi_n(x) = (2^n n! \sqrt{\pi})^{-1/2} H_n(x) e^{-x^2/2}, \quad (\text{A.12})$$

where  $H_n(x)$  is the usual Hermite polynomial.

A well-known method for finding the eigenfunctions of  $H_{\text{HO}}$  in one dimension involves writing

$$H_{\text{HO}} = a^\dagger a + \frac{1}{2}, \quad (\text{A.13})$$

where the ladder operator  $a$  is given by

$$a \equiv \frac{1}{\sqrt{2}}(x + \partial_x), \quad (\text{A.14})$$

with Hermitian adjoint  $a^\dagger$  given by

$$a^\dagger \equiv \frac{1}{\sqrt{2}}(x - \partial_x). \quad (\text{A.15})$$

The name “ladder operator” comes from the important formulas

$$a\phi_n(x) = \sqrt{n}\phi_{n-1}(x) \quad (\text{A.16})$$

$$a^\dagger\phi_n(x) = \sqrt{n+1}\phi_{n+1}(x), \quad (\text{A.17})$$

valid for all  $n$ . This can easily be proved by using the recurrence relation (2.7). By repeatedly acting on  $\phi_0$  with  $a^\dagger$  we generate every Hermite function, viz,

$$\phi_n(x) = n!^{-1/2}(a^\dagger)^n\phi_0(x). \quad (\text{A.18})$$

As Hermite functions constitute a complete, orthonormal sequence in  $L^2(\mathbb{R})$ , any  $\psi \in L^2(\mathbb{R})$  can be written as a series in Hermite functions, viz,

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x), \quad (\text{A.19})$$

where the coefficients  $c_n$  are uniquely determined by  $c_n = \langle \phi_n, \psi \rangle$ .

An interesting fact is that the Hermite functions are also eigenfunctions of the Fourier transform with eigenvalues  $(-i)^n$ , as can easily be proved by induction by observing firstly that the Fourier transform of  $\phi_0(x)$  is  $\phi_0(k)$  itself, and secondly that the Fourier transform of  $a^\dagger$  is  $-ia^\dagger$  (acting on the variable  $y$ ). It follows from completeness of the Hermite functions, that the Fourier transform defines a unitary operator on  $L^2(\mathbb{R})$ .

We now make a simple observation, namely that

$$(a^\dagger)^k \phi_n(x) = P_k(n)^{1/2} \phi_{n+k}(x), \quad (\text{A.20})$$

where  $P_k(n) = (n+k)!/n! > 0$  is a polynomial of degree  $k$  for  $n \geq 0$ . Moreover  $P_k(n+1) > P_k(n)$  and  $P_{k+1}(n) > P_k(n)$ .

We now prove the following lemma:

**Lemma 1 (Hermite series in one dimension)**

Let  $\psi \in L^2(\mathbb{R})$ . Then

1.  $a^\dagger\psi \in L^2(\mathbb{R})$  if and only if  $a\psi \in L^2(\mathbb{R})$  if and only if  $\sum_{n=0}^{\infty} n|c_n|^2 < +\infty$ , where  $c_n = \langle \phi_n, \psi \rangle$
2.  $a^\dagger\psi \in L^2(\mathbb{R})$  if and only if  $x\psi, \partial_x\psi \in L^2(\mathbb{R})$

3.  $(a^\dagger)^{k+1}\psi \in L^2(\mathbb{R})$  implies  $(a^\dagger)^k\psi \in L^2(\mathbb{R})$

4.  $(a^\dagger)^k\psi \in L^2(\mathbb{R})$  if and only if

$$\sum_{n=0}^{\infty} n^k |c_n|^2 < +\infty. \quad (\text{A.21})$$

5.  $(a^\dagger)^k\psi \in L^2(\mathbb{R})$  if and only if  $x^j \partial_x^{k-j}\psi \in L^2(\mathbb{R})$  for  $0 \leq j \leq k$

*Proof:* We have

$$\|a^\dagger\psi\|^2 = \sum_{n=0}^{\infty} (n+1)|c_n|^2 = \|\psi^2\| + \|a\psi\|^2, \quad (\text{A.22})$$

from which statement 1 follows. Statement 2 follows from the definition of  $a^\dagger$ , and that  $a^\dagger\psi \in L^2$  implies  $a\psi \in L^2$  (since  $\|a\psi\| \leq \|a^\dagger\psi\|$ ), which again implies  $x\psi, \partial_x\psi \in L^2$ . Statement 3 follows from the monotone behaviour of  $P_k(n)$  as function of  $k$ . Statement 4 then follows. By iterating statement 2 and using  $[\partial_x, x] = 1$  and statement 3, statement 5 follows.  $\diamond$

The significance of the condition  $a^\dagger\psi \in L^2(\mathbb{R})$  is that the coefficients  $c_n$  of  $\psi$  must decay faster than for a completely arbitrary wave function in  $L^2(\mathbb{R})$ . Moreover,  $a^\dagger\psi \in L^2(\mathbb{R})$  is the same as requiring  $\partial_x\psi \in L^2(\mathbb{R})$ , and  $x\psi \in L^2(\mathbb{R})$ . Lemma 1 also generalizes this fact for  $(a^\dagger)^k\psi \in L^2(\mathbb{R})$ , giving successfully quicker decay of the coefficients. In all cases, the decay is expressed in an average sense, through a growing weight function in a sum, as in Eqn. (A.21). Since the terms in the sum must converge to zero, this implies a pointwise faster decay, as stated in Eqn. (A.25) below.

We comment here, that the partial derivatives must be understood in the weak, or distributional, sense: Even though  $\psi$  may not be everywhere differentiable in the ordinary sense, it may have a weak derivative. For example, if the classical derivative exists everywhere except for a countable set (and if it is in  $L^2$ ), this is the weak derivative. Moreover, if this derivative has a jump discontinuity, there are no higher order weak derivatives.

Loosely speaking, since  $x\psi(x) \in L^2 \Leftrightarrow \partial_y\hat{\psi}(y) \in L^2$ , where  $\hat{\psi}(y)$  is the Fourier transform, point 2 of Lemma 1 is a combined smoothness condition on  $\psi(x)$  and  $\hat{\psi}(y)$ . Point 5 is a generalization to higher derivatives, but is difficult to check in general for an arbitrary  $\psi$ . On the other hand, it is well-known that the eigenfunctions of many Hamiltonians of interest, such as the quantum dot Hamiltonian (2.15), decay exponentially fast as  $|x| \rightarrow \infty$ . For such exponentially decaying functions over  $\mathbb{R}^1$ ,  $x^k\psi \in L^2(\mathbb{R})$  for all  $k \geq 0$ , i.e.,  $\hat{\psi}(y)$  is infinitely differentiable. We then have the following lemma:

**Lemma 2 (Exponential decay in 1D)**

Assume that  $x^k\psi \in L^2(\mathbb{R})$  for all  $k \geq 0$ . Then a sufficient criterion for  $(a^\dagger)^m\psi \in L^2(\mathbb{R})$  is  $\partial_x^m\psi \in L^2(\mathbb{R})$ , i.e.,  $\psi \in H^m(\mathbb{R})$ . In fact,  $x^k\partial_x^{m'}\psi \in L^2$  for all  $m' < m$  and all  $k \geq 0$ .

*Proof:* We prove the Proposition inductively. We note that, since  $\partial_x^m \psi \in L^2$  implies  $\partial_x^{m-1} \psi \in L^2$ , the proposition holds for  $m-1$  if it holds for a given  $m$ . Moreover, it holds trivially for  $m=1$ .

Assume then, that it holds for a given  $m$ , i.e., that  $\psi \in H^m$  implies  $x^k \partial_x^{m-j} \psi \in L^2$  for  $1 \leq j \leq m$  and for all  $k$  (so that, in particular,  $(a^\dagger)^m \psi \in L^2$ ). It remains to prove, that  $\psi \in H^{m+1}$  implies  $x^k \partial_x^m \psi \in L^2$ , since then  $(a^\dagger)^{m+1} \psi \in L^2$  by statement 5 of Lemma 1. We compute the norm and use integration by parts, viz,

$$\begin{aligned} \|x^k \partial_x^m \psi\|^2 &= \int_{\mathbb{R}} x^{2k} \partial_x^k \psi^*(x) \partial_x^k \psi(x) \\ &= -2k \langle \partial_x^m \psi, x^{2k-1} \partial_x^{m-1} \psi \rangle \\ &\quad - \langle \partial_x^{m+1} \psi, x^{2k} \partial_x^{m-1} \psi \rangle < +\infty. \end{aligned}$$

The boundary terms vanish. Therefore,  $x^k \partial_x^m \psi \in L^2$  for all  $k$ , and the proof is complete.  $\diamond$

The proposition states that for the subset of  $L^2(\mathbb{R})$  consisting of exponentially decaying functions, the approximation properties of the Hermite functions will *only* depend on the smoothness properties of  $\psi$ . Moreover, the derivatives up to the penultimate order decay exponentially as well. (The highest order derivative may decay much slower.)

From Lemmas 1 and 2 we extract the following important characterization of the approximating properties of Hermite functions in  $d=1$  dimensions:

**Proposition 1 (Approximation in one dimension)**

Let  $k \geq 0$  be a given integer. Let  $\psi \in L^2(\mathbb{R})$  be given by

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x). \quad (\text{A.23})$$

Then  $\psi \in H^k(\mathbb{R})$  if and only if

$$\sum_{n=0}^{\infty} n^k |c_n|^2 < \infty. \quad (\text{A.24})$$

The latter implies that

$$|c_n| = o(n^{-(k+1)/2}). \quad (\text{A.25})$$

Let  $\psi_R = P_R \psi = \sum_{n=0}^R c_n \phi_n$ . Then

$$\|\psi - \psi_R\| = \left( \sum_{n=R+1}^{\infty} |c_n|^2 \right)^{1/2}. \quad (\text{A.26})$$

This is the central result for Hermite series approximation in  $L^2(\mathbb{R}^1)$ . Observe that Eqn. (A.25) implies that the error  $\|\psi - \psi_R\|$  can easily be estimated. See also Prop. 2 and comments thereafter.

Now a word on pointwise convergence of the Hermite series. As the Hermite functions are uniformly bounded,<sup>25</sup> viz,

$$|\phi_n(x)| \leq 0.816 \quad \forall x \in \mathbb{R}, \quad (\text{A.27})$$

the pointwise error in  $\psi_R$  is bounded by

$$|\psi(x) - \psi_R(x)| \leq 0.816 \sum_{n=R+1}^{\infty} |c_n|. \quad (\text{A.28})$$

Hence, if the sum on the right hand side is finite, the convergence is uniform. If the coefficients  $c_n$  decay rapidly enough, both errors can be estimated by the dominating neglected coefficients.

We now consider expansions of functions in  $L^2(\mathbb{R}^n)$ . To stress that  $\mathbb{R}^n$  may be other than the configuration space of a single particle, we use the notation  $x = (x_1, \dots, x_n) \in \mathbb{R}^n$  instead of  $\vec{r} \in \mathbb{R}^d$ . For  $N$  electrons in  $d$  spatial dimensions,  $n = Nd$ .

Recall that the Hermite functions over  $\mathbb{R}^n$  are indexed by multi-indices  $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathcal{I}_n$ , and that

$$\Phi_\alpha(x) \equiv \phi_{\alpha_1}(x_1) \cdots \phi_{\alpha_n}(x_n). \quad (\text{A.29})$$

Now, to each spatial coordinate  $x_k$  define the ladder operators  $a_k \equiv (x_k + \partial_k)/\sqrt{2}$ . These obey  $[a_j, a_k] = 0$  and  $[a_j, a_k^\dagger] = \delta_{j,k}$ , as can easily be verified. Let  $\mathbf{a}$  be a formal vector of the ladder operators, viz,

$$\mathbf{a} \equiv (a_1, a_2, \dots, a_n). \quad (\text{A.30})$$

For the first Hermite function, we have

$$\Phi_0(x) \equiv \pi^{-n/4} e^{-\|x\|^2/2}. \quad (\text{A.31})$$

By using Eqn. (A.18) and Eqn. (A.4), we may generate all other Hermite functions, viz,

$$\Phi_\alpha(x) \equiv \alpha!^{-1/2} (\mathbf{a}^\dagger)^\alpha \Phi_0(x). \quad (\text{A.32})$$

Given two multi-indices  $\alpha$  and  $\beta$ , we define the polynomial  $P_\alpha(\beta)$  by

$$P_\beta(\alpha) \equiv \frac{(\alpha + \beta)!}{\alpha!} = \prod_{j=1}^D P_{\beta_j}(\alpha_j), \quad (\text{A.33})$$

where  $P$  is defined for integers as before.

Since the Hermite functions  $\Phi_\alpha$  constitute a basis, any  $\psi \in L^2(\mathbb{R}^n)$  can be expanded as

$$\psi(x) = \sum_{\alpha} c_{\alpha} \Phi_{\alpha}(x), \quad \|\psi\|^2 = \sum_{\alpha} |c_{\alpha}|^2, \quad (\text{A.34})$$

where the sum is to be taken over all multi-indices  $\alpha \in \mathcal{I}_n$ . Now, let  $\beta \in \mathcal{I}_n$  be arbitrary. By using Eqn. (A.17) in each spatial direction we compute the action of  $(\mathbf{a}^\dagger)^\beta$  on  $\psi$ :

$$\begin{aligned} (\mathbf{a}^\dagger)^\beta \psi &= (a_1^\dagger)^{\beta_1} \cdots (a_n^\dagger)^{\beta_n} \sum_{\alpha} c_{\alpha} \Phi_{\alpha} \\ &= \sum_{\alpha} c_{\alpha} \prod_{k=1}^n \frac{(\alpha_k + \beta_k)!^{1/2}}{\alpha_k!^{1/2}} \Phi_{\alpha+\beta} \\ &= \sum_{\alpha} c_{\alpha} P_{\beta}(\alpha)^{1/2} \Phi_{\alpha+\beta}. \end{aligned} \quad (\text{A.35})$$

Similarly, by using Eqn. (A.16) we obtain

$$\begin{aligned} \mathbf{a}^\beta \psi &= a_1^{\beta_1} \cdots a_n^{\beta_n} \sum_{\alpha} c_{\alpha} \Phi_{\alpha} \\ &= \sum_{\alpha} c_{\alpha+\beta} \prod_{k=1}^n \frac{(\alpha_k + \beta_k)!^{1/2}}{\alpha_k!^{1/2}} \Phi_{\alpha} \\ &= \sum_{\alpha} c_{\alpha+\beta} P_{\beta}(\alpha)^{1/2} \Phi_{\alpha}, \end{aligned} \quad (\text{A.36})$$

Computing the square norm gives

$$\|(\mathbf{a}^\dagger)^\beta \psi\|^2 = \sum_{\alpha} P_{\beta}(\alpha) |c_{\alpha}|^2. \quad (\text{A.37})$$

and

$$\|\mathbf{a}^\beta \psi\|^2 = \sum_{\alpha} P_{\beta}(\alpha) |c_{\alpha+\beta}|^2. \quad (\text{A.38})$$

The polynomial  $P_{\beta}(\alpha) > 0$  for all  $\beta, \alpha \in \mathcal{I}_n$ , and  $P_{\beta}(\alpha + \alpha') > P_{\beta}(\alpha)$  for all non-zero multi-indices  $\alpha' \neq 0$ . Therefore, if  $(\mathbf{a}^\dagger)^\beta \psi \in L^2(\mathbb{R}^n)$  then  $\mathbf{a}^\beta \psi \in L^2(\mathbb{R}^n)$ . However, the converse is not true for  $n > 1$  dimensions, as the norm in Eqn. (A.38) is independent of infinitely many coefficients  $c_{\alpha}$ , while Eqn. (A.37) is not. (This should be contrasted with the one-dimensional case, where  $a\psi \in L^2(\mathbb{R})$  was equivalent to  $a^\dagger \psi \in L^2(\mathbb{R})$ .) On the other hand, as in the  $n = 1$  case, the condition  $a_k^\dagger \psi \in L^2(\mathbb{R}^n)$  is equivalent to the conditions  $x_k \psi \in L^2(\mathbb{R}^n)$  and  $\partial_k \psi \in L^2(\mathbb{R}^n)$ .

We are in position to formulate a straightforward generalization of Lemma 1. The proof is easy, so we omit it.

### Lemma 3 (General Hermite expansions)

Let  $\psi \in L^2(\mathbb{R}^n)$ , with coefficients  $c_{\alpha}$  as in Eqn. (A.34), and let  $\beta \in \mathcal{I}_n$  be arbitrary. Assume  $(\mathbf{a}^\dagger)^\beta \psi \in L^2(\mathbb{R}^n)$ . Then  $(\mathbf{a}^\dagger)^{\beta'} \psi \in L^2(\mathbb{R}^n)$  and  $\mathbf{a}^{\beta'} \psi \in L^2(\mathbb{R}^n)$  for all  $\beta' \leq \beta$ . Moreover, the following points are equivalent:

1.  $(\mathbf{a}^\dagger)^\beta \psi \in L^2(\mathbb{R}^n)$
2. For all multi-indices  $\gamma \leq \beta$ ,  $x^\gamma \partial^{\beta-\gamma} \psi \in L^2(\mathbb{R}^n)$ .
3.  $\sum_{\alpha} \alpha^\beta |c_{\alpha}|^2 < +\infty$

We observe, that as we obtained for  $n = 1$ , condition 2 is a combined decay and smoothness condition on  $\psi$ , and that this can be expressed as a decay-condition on the coefficients of  $\psi$  in the Hermite basis by 3.

Exponential decay of  $\psi \in L^2(\mathbb{R}^n)$  as  $\|x\| \rightarrow \infty$  implies that  $x^\gamma \psi \in L^2(\mathbb{R}^n)$  for all  $\gamma \in \mathcal{I}_n$ . We now generalize Lemma 2 to the  $n$ -dimensional case.

### Lemma 4 (Exponentially decaying functions)

Assume that  $\psi \in L^2(\mathbb{R}^n)$  is such that for all  $\gamma \in \mathcal{I}_n$ ,  $x^\gamma \psi \in L^2(\mathbb{R}^n)$ . Then, a sufficient criterion for  $(\mathbf{a}^\dagger)^\beta \psi \in L^2(\mathbb{R}^n)$  is  $\partial^\beta \psi \in L^2(\mathbb{R}^n)$ . Moreover, for all  $\mu \leq \beta$ , we have  $x^\gamma \partial^{\beta-\mu} \psi \in L^2(\mathbb{R}^n)$  for all  $\gamma \in \mathcal{I}_n$  such that  $\gamma_k = 0$  whenever  $\mu_k = 0$ , i.e., the partial derivatives of lower order than  $\beta$  decay exponentially in the directions where the differentiation order is lower.

*Proof:* The proof is a straightforward application of the  $n = 1$  case in an inductive proof, together with the following elementary fact concerning weak derivatives: If  $1 \leq j < k \leq n$ , and if  $x_j \psi(x)$  and  $\partial_k \psi(x)$  are in  $L^2(\mathbb{R}^n)$ , then, by the product rule,  $\partial_k(x_j \psi(x)) = x_j(\partial_k \psi(x)) \in L^2(\mathbb{R}^n)$ . Notice, that Lemma 2 trivially generalizes to a single index in  $n$  dimensions, i.e., to  $\beta = \beta_k e_k$ , since the integration by parts formula used is valid in  $\mathbb{R}^n$  as well. Similarly, the present Lemma is valid in  $n - 1$  dimensions if it holds in  $n$  dimensions, as it must be valid for  $\beta = (0, \beta_2, \dots, \beta_n)$ .

Assume that our statement holds for  $n - 1$  dimensions. We must prove that it then holds in  $n$  dimensions. Assume then, that  $\partial^\beta \psi \in L^2(\mathbb{R}^n)$ . Let  $\phi = \partial^{\bar{\beta}} \psi \in L^2$ . Moreover,  $\partial_1^{\beta_1} \phi \in L^2$ . Since  $\psi$  is exponentially decaying, and by the product rule,  $x_1^{\gamma_1} \phi \in L^2$  for all  $\gamma_1 \geq 0$ . By Lemma 2,  $x_1^{\gamma_1} \partial_1^{\beta_1 - \mu_1} \phi \in L^2$  for all  $\gamma_1$  and  $0 < \mu_1 \leq \beta_1$ . Thus,  $x_1^{\gamma_1} \partial^{\beta - e_1 \mu_1} \psi \in L^2$ . Thus, the result holds as long as  $\mu = e_1 \mu_1$ ; or equivalently  $\mu = e_k \mu_k$  for any  $k$ . To apply induction, let  $\chi = x_1^{\gamma_1} \partial_1^{\beta_1 - \mu_1} \psi \in L^2$ . Note that  $\partial^{\bar{\beta}} \chi \in L^2$  and  $x^{\bar{\gamma}} \chi \in L^2$  for all  $\bar{\gamma} = (0, \gamma_2, \dots, \gamma_n)$ . But by the induction hypothesis,  $x^{\bar{\gamma}} \partial^{\bar{\beta} - \bar{\mu}} \chi \in L^2$  for all  $\bar{\mu} \leq \bar{\beta}$  and all  $\bar{\gamma}$  such that  $\bar{\gamma}_k = 0$  if  $\bar{\mu}_k = 0$ . This yields, using the product rule, that  $x^{\bar{\gamma}} \partial^{\beta - \mu} \psi \in L^2$  for all  $\mu \leq \beta$  and all  $\bar{\gamma}$  such that  $\gamma_k = 0$  if  $\mu_k = 0$ , which was the hypothesis for  $n$  dimensions, and the proof is complete. Notice, that we have proved that  $(\mathbf{a}^\dagger)^\beta \psi \in L^2$  as a by-product.  $\diamond$

In order to generate a simple and useful result for approximation in  $n$  dimensions, we consider the case where  $\psi$  decays exponentially, and  $\psi \in H^k(\mathbb{R}^n)$ , i.e.,  $\partial^\beta \psi(x) \in L^2(\mathbb{R}^n)$  for all  $\beta \in \mathcal{I}_n$  with  $|\beta| = k$ . In this case, we may also generalize Eqn. (A.25). For this, we consider the shell-weight  $p(r)$  defined by

$$p(r) \equiv \sum_{\alpha \in \mathcal{I}_n, |\alpha|=r} |c_{\alpha}|^2, \quad (\text{A.39})$$

where  $c_{\alpha} = \langle \Phi_{\alpha}, \psi \rangle$ . Then,  $\|\psi\|^2 = \sum_{r=0}^{\infty} p(r)$ . Moreover, if  $P$  projects onto the shell-truncated Hilbert space  $\mathcal{P}_R(\mathbb{R}^n)$ , then

$$\|P\psi\|^2 = \sum_{r=0}^R p(r). \quad (\text{A.40})$$

### Proposition 2 (Approximation in $n$ dimensions)

Let  $\psi \in L^2(\mathbb{R}^n)$  be exponentially decaying and given by

$$\psi(x) = \sum_{\alpha} c_{\alpha} \Phi_{\alpha}(x). \quad (\text{A.41})$$

Then  $\psi \in H^k(\mathbb{R}^n)$ ,  $k \geq 0$ , if and only if

$$\sum_{\alpha} |\alpha|^k |c_{\alpha}|^2 = \sum_{r=0}^{\infty} r^k p(r) < +\infty. \quad (\text{A.42})$$

The latter implies that

$$p(r) = o(r^{-(k+1)}). \quad (\text{A.43})$$



Moreover, for the shell-truncated Hilbert space  $\mathcal{P}_R$ , the approximation error is given by

$$\|(1-P)\psi\| = \left( \sum_{r=R+1}^{\infty} p(r) \right)^{1/2}. \quad (\text{A.44})$$

*Proof:* The only non-trivial part of the proof concerns Eqn. (A.42). Since  $\psi$  is exponentially decaying and since  $\psi \in H^k$  if and only if  $\partial^\beta \psi \in L^2$  for all  $\beta$ ,  $|\beta| \leq k$ , we know that  $\sum_{\alpha} \alpha^\beta |c_\alpha|^2 < +\infty$  for all  $\beta$ ,  $|\beta| \leq k$ . Since

$|\alpha|^k$  is a polynomial of order  $k$  with terms of type  $a_\beta \alpha^\beta$ ,  $a_\beta \geq 0$  and  $|\beta| = k$ , we have

$$\sum_{\alpha} |\alpha|^k |c_\alpha|^2 = \sum_{\beta, |\beta|=k} a_\beta \sum_{\alpha} \alpha^\beta |c_\alpha|^2 < +\infty. \quad (\text{A.45})$$

On the other hand, since  $a_\beta \geq 0$  and the sum over  $\beta$  has finitely many terms,  $\sum_{\alpha} |\alpha|^k |c_\alpha|^2 < +\infty$  implies  $\sum_{\alpha} \alpha^\beta |c_\alpha|^2 < +\infty$  for all  $\beta$ ,  $|\beta| = k$ , and thus  $\psi \in H^k$  since  $\psi$  was exponentially decaying.  $\diamond$

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